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1996 J. Phys.: Condens. Matter 8 1051

(http://iopscience.iop.org/0953-8984/8/8/015)

J. Phys.: Condens. Matter **8** (1996) 1051–1058. Printed in the UK

Soliton propagation in a classical Heisenberg chain with impurities

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Received 11 September 1995, in final form 24 November 1995

Abstract. We present numerical studies of soliton propagation in a classical Heisenberg chain which contains a disordered binary-alloy segment having impurities of spin different from that of the host with density p. It is demonstrated that the reflected and the transmitted solitons exhibit robust features. The transmission coefficient decreases with increasing soliton energy in the range investigated, and displays a long-tail power-law length dependence with an exponent close to -1. It is also shown that the impurity bonds, which connect neighbouring sites with different spins, are the elementary scattering units which lead to wave interferences important for the soliton propagation.

1. Introduction

During the last two decades there has been a great deal of interest in the problem of spin-wave propagation in disordered Heisenberg spin chains [1–4]. Usually the spin waves are considered within the one-magnon approximation which ignores the nonlinear terms in the Hamiltonian. On the other hand the effect of nonlinearity in low-dimensional homogeneous Heisenberg Hamiltonian systems has also been extensively investigated [5–10]. It was revealed that nonlinear terms in the Hamiltonian may lead to stable soliton propagation. For example, the one-dimensional classical Heisenberg system is completely integrable and the soliton solutions can be explicitly obtained [7–10]. The interplay between disorder and nonlinearity in these systems is an important subject and has drawn much attention in recent years [11–14].

Since the solitons in a classical Heisenberg chain described in [10] have a well-defined form, they may serve as a good starting point for the study of the effect of disorder. The purpose of this paper is to consider how solitons propagate in a disordered segment with impurity spins and to obtain the behaviour of the transmission coefficient as a function of the soliton energy and the length of the segment. We have performed computer experiments on the propagation of solitons in such a system and calculated the corresponding transmission coefficient. We find that the reflected and the transmitted solitons exhibit robust features. Moreover, the transmission coefficient decreases with increasing soliton energy in the range investigated, and displays a long-tail power-law length dependence with an exponent close to -1. The elementary units which are responsible for the soliton scattering are also pointed out and the interference effects are analysed from the results obtained.

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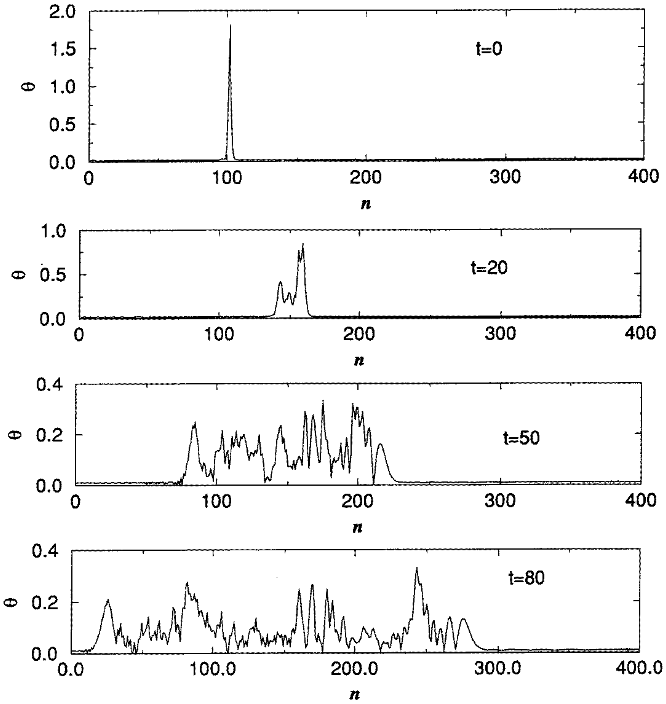
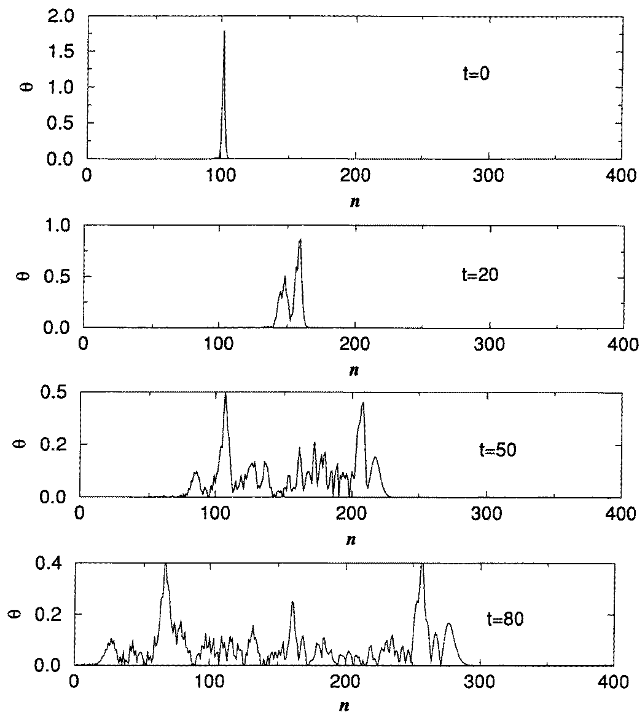
0953-8984/96/081051+08$19.50

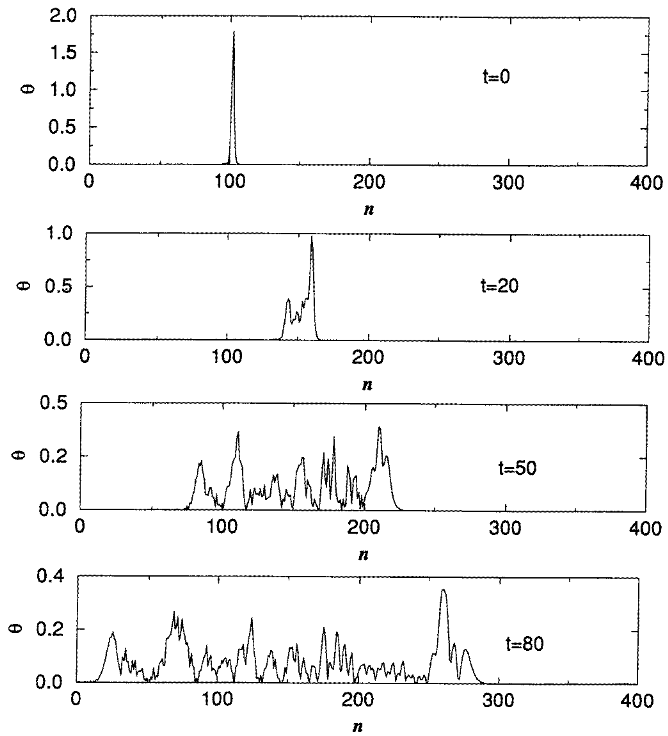


(a)



(b)

Figure 1. See facing page for caption.



(c)

Figure 1. (Continued.) (a) The propagation of a soliton with energy $\epsilon = 1.5$ and velocity 1.416 in a classical Heisenberg chain of spin 1 with an inserted disordered segment which contains impurity sites of spin $s = 2$ of concentration $p = 0.6$. The length of the chain is 400; the disordered segment has $L = 50$ sites and is situated from the site $n = 175$ to the site $n = 225$. (b) The propagation of a soliton in a chain with the same parameters as in (a) except for the spin impurity density in the segment, which is now $p = 0.3$. (c) The same as (a) but with the spin impurity density $p = 0.9$.

2. Model and formalism

A classical Heisenberg spin chain with nearest-neighbour exchange interactions can be expressed by the Hamiltonian [10]

$$H = -\sum_n \ln(G_{n,n+1}) \tag{1}$$

where n labels the lattice sites and

$$G_{n,n+1} = 1 + J_{n,n+1}\boldsymbol{s}_n \cdot \boldsymbol{s}_{n+1}.$$

Here $\boldsymbol{s}_n$ is a unit vector and the coupling strength is assumed to be

$$J_{n,n+1} = \frac{2\mu_n\mu_{n+1}}{\mu_n^2 + \mu_{n+1}^2} \tag{2}$$

where μ_n is a parameter describing the spin at site n. In this representation we have

$$G_{n,n+1} = 1 + J_{n,n+1}[\cos(\theta_n)\cos(\theta_{n+1}) + \cos(\phi_n - \phi_{n+1})\sin(\theta_n)\sin(\theta_{n+1})]$$

with θ_n and ϕ_n the polar-coordinate angles of the spin orientation. The equations of motion for the nth spin are

$$\sin(\theta_n)\dot{\phi}_n = -\frac{\partial H}{\partial \theta_n} \qquad \sin(\theta_n)\dot{\theta}_n = \frac{\partial H}{\partial \phi_n} \tag{3}$$

which can be explicitly expressed as

$$\begin{aligned}\frac{\partial H}{\partial \theta_n} = &-\frac{J_{n,n+1}}{G_{n,n+1}}[-\sin\theta_n \cos\theta_{n+1} + \cos(\phi_n - \phi_{n+1})\cos\theta_n \sin\theta_{n+1}] \\ &-\frac{J_{n-1,n}}{G_{n-1,n}}[-\cos\theta_{n-1}\sin\theta_n + \cos(\phi_n - \phi_{n-1})\sin\theta_{n-1}\cos\theta_n]\end{aligned} \tag{4}$$

$$\frac{\partial H}{\partial \phi_n} = \frac{J_{n,n+1}}{G_{n,n+1}}\sin(\phi_n - \phi_{n+1})\sin\theta_n \sin\theta_{n+1} + \frac{J_{n-1,n}}{G_{n-1,n}}\sin(\phi_n - \phi_{n-1})\sin\theta_{n-1}\sin\theta_n. \tag{5}$$

For a homogeneous system with $\mu_n = 1$ for all n the above equations are completely integrable, giving the soliton solution [10]

$$\cos\theta_n = 1 - \frac{\Gamma}{\Xi_n} \tag{6}$$

$$\begin{aligned}\phi_n = \phi_0 + \sigma n &+ (\cos\sigma \cosh\epsilon - 1)t \\ &+ \tan^{-1}\left[\frac{\tanh(\epsilon/2)}{\tan(\sigma/2)}\tanh(\epsilon n - (\sinh\epsilon)(\sin\sigma)t - x_0)\right]\end{aligned} \tag{7}$$

where

$$\begin{aligned}\Gamma &\equiv \frac{\sinh^2\epsilon}{\cosh\epsilon - \cos\sigma} \\ \Xi_n &= \cosh\left[\epsilon\left(n + \frac{1}{2}\right) - (\sinh\epsilon)(\sin\sigma)t - x_0\right] \\ &\quad \times \cosh\left[\epsilon\left(n - \frac{1}{2}\right) - (\sinh\epsilon)(\sin\sigma)t - x_0\right].\end{aligned} \tag{8}$$

The parameters ϵ, ϕ_0 and x_0 are the energy, the initial azimuthal orientation and the position of the soliton, respectively, while the velocity of the soliton is $(\sin\sigma)(\sinh\epsilon)/\epsilon$.

Now we insert a disordered segment into a homogeneous chain with spin $\mu = 1$. The segment is a binary alloy consisting of impurity sites of spin $\mu = s \neq 1$ with probability p and host sites of spin 1 with probability $1 - p$. A kink soliton in the form of equations (6) and (7) is incident on the disordered segment from the left-hand part of the homogeneous chain and our purpose is to see how the soliton propagates through the disordered segment. As the equations of motion are no longer integrable, we perform computer experiments to solve them for various choices of the soliton energy, the impurity concentration and the length of the segment.

3. Numerical results

We use the fourth-order Runge–Kutta method to solve the equations of motion for a system involving 400 sites with periodic boundary conditions at the two ends of the chain. The accuracy of the calculations is controlled by choosing the time step of the Runge–Kutta procedure to be small enough that the relative error of the total energy from its exact value was less than 0.001 in all of the cases examined. From the data obtained we can compute the transmission coefficient of a soliton as a function of its energy and the segment length.

In figure 1(a) we display a soliton propagating with energy $\epsilon = 1.5$ and velocity $\sigma = 1.5$ in a classical Heisenberg chain of spin 1, with a disordered segment of length $L = 50$ which contains impurity sites of spin $s = 2$ with concentration $p = 0.6$. As is expected, before the soliton peak encounters the segment it propagates steadily. Upon scattering by the impurities the soliton is shown to decompose into three parts: the transmitted part, the reflected part, and a ripple remaining in the segment. These parts persist in the kink form and no anti-kink solitons appear. It should also be pointed out that this behaviour is clearly different from the corresponding propagation of vibrational solitons in nonlinear chains in the presence of impurities [11], where a kink soliton decomposes into kink and anti-kink parts after scattering. Moreover, after a long time the peaks in the transmitted or in the reflected parts tend to gather together, forming a single soliton moving in the homogeneous chain, while the ripple slowly comes out of the disordered segment to join the reflected and the transmitted parts.

The soliton propagation becomes slightly different when we change the concentration of the impurities. In figures 1(b) and 1(c) we plot the propagation of the same soliton in a chain with a disordered segment of the same length but with different impurity spin concentrations ($p = 0.3$ and $p = 0.9$). The soliton again decomposes into three parts upon scattering, but the detailed structures of the transmitted and reflected solitons as well as the ripples now slightly change, indicating different effects of interference between the waves scattered by the impurities.

From the equations of motion considered it can be easily seen that if the segment consists of only one type of impurity spin ($p = 1.0$), if its length is larger than the corresponding soliton scale, the soliton keeps its shape and its velocity, no matter how different the spins are in the segment and the host. To illustrate this point, in figure 2 we plot the propagation of a soliton in a chain with a homogeneous segment, i.e. with all the spins in it being the same but different from the spin of the host. In this case it is seen that the soliton is scattered only at the interfaces between two spins and remains unchanged within the segment. In fact, in the equations of motion the spin values only appear in pairs of nearest-neighbour sites. Since there exist a large number of such impurity bonds, the waves generated by them are repeatedly reflected by each other, and due to this complicated process a ripple is naturally created.

We have calculated the transmission coefficient $T(\epsilon)$, defined as the ratio of the transmitted energy to the total energy, to obtain the dependences of the transmission on the energy ($T(\epsilon)$), and the length ($T(L)$) of the segment. In order to reveal the relevance of the impurity bonds in the soliton scattering we calculate the energy dependence of the transmission coefficient for a system containing only two impurity bonds ($L = 1$) and compare the results with those for the case of a disordered segment of length $L = 50$ with concentration $p = 0.6$. The energy dependences of the transmission are plotted in figure 3 for the two cases. We can see that $T(\epsilon)$ decreases when the energy of the incident soliton increases, in analogy with previous results for the nonlinear disordered elastic chains [12]. We also notice that the amplitude of the transmitted soliton approaches zero at almost the same value of ϵ for the single impurity bond and the full segment. This implies that in the high-reflection limit the soliton is almost reflected at the first impurity bond encountered and the rest of the bonds have no effect on its propagation. The data obtained can be approximately fitted with the function

$$T(\epsilon) = 1 - c\epsilon^{\alpha} \tag{9}$$

with parameters c and α. In the case of a single impurity bond we obtain $\alpha \approx 4.6$, $c \approx 0.042$, with the total fitting variance $\Delta^2 \approx 0.07$, and in the case of the impurity segment $\alpha \approx 2.9$,

$c \approx 0.13$, with a variance $\Delta^2 \approx 0.02$. It must be pointed out that the exponent α has no specific physical meaning, since it must vary with the length, the spin value and the concentration of the impurities.

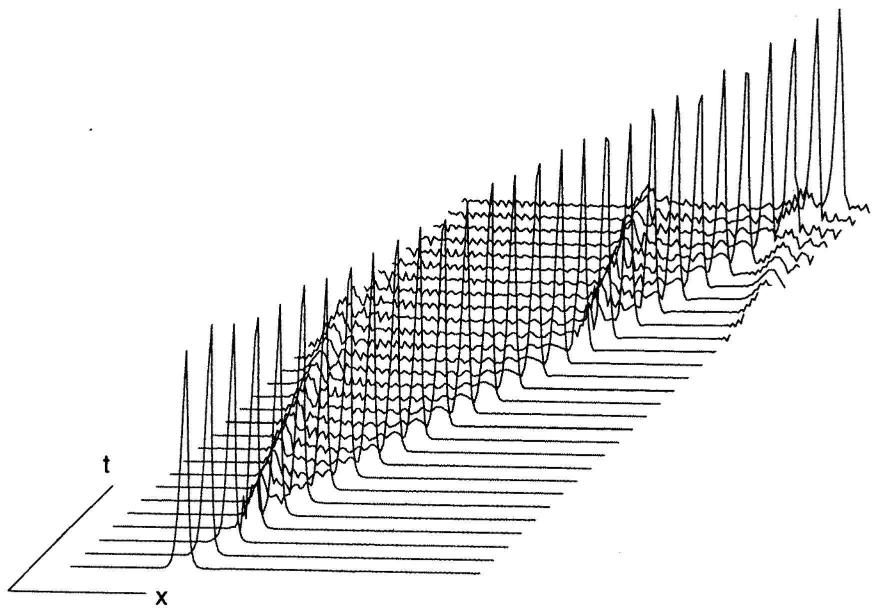


Figure 2. Space-time evolution of a soliton through a homogeneous segment with spin $s = 2$, different from that of the host.

Figure 3 also shows that in the case of weak reflection the coefficient of transmission through the disordered segment is smaller than that via a single impurity bond, because of the multi-scattering process in the former case. If there were no interference effects in this process, the transmission coefficient $T(L)$ would display an exponential decay as a function of the length of the disordered segment L. We have calculated the length dependence of $T(L)$ for the propagation of a soliton with energy $\epsilon = 1.625$ through the segment with impurity density $p = 0.6$. The results plotted in figure 4 with log–log scales can also be fitted to a power law

$$T(\epsilon) = bL^{\mu} \tag{10}$$

with $\mu \approx -0.98$, $b \approx 4.3$, with a variance $\Delta^2 \approx 0.003$. Therefore, the transmission coefficient does not decay exponentially but shows a long-tail behaviour characterized by an exponent close to -1, which is due to the presence of strong interference effects. This also implies that the waves scattered from different impurity bonds are strongly correlated, a fact that has already been recognized in the soliton structures and the ripples in figures 1(a)–1(c). The corresponding exponent μ derived for the elastic chains using a linear wave transmission approximation in [12] is $-1/2$ for a quartic potential and is $-3/2$ for a cubic potential. The difference of our μ from these values is attributed partly to the special form of the potential in the model studied and partly to the strong interference effects. Earlier investigations on the damping of solitons in a sine–Gordon chain also demonstrated the interference effects on phase locking [13, 14].

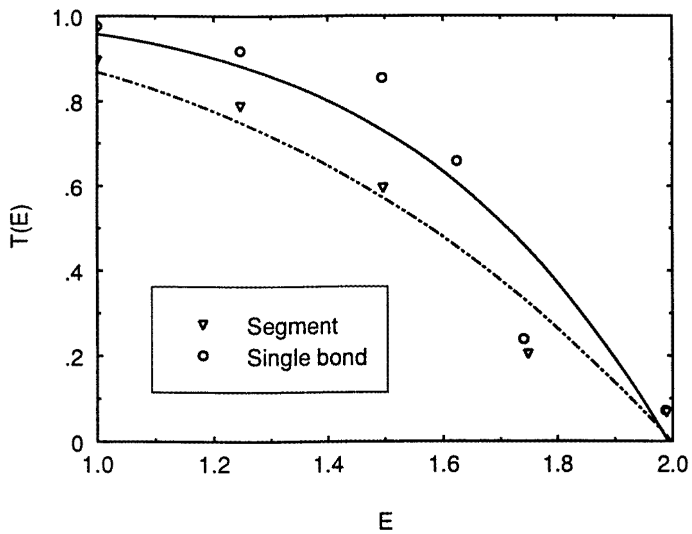


Figure 3. The relation between the transmission coefficient and the energy for a soliton propagating through an impurity segment and through a single impurity bond. The curves represent the fitting functions.

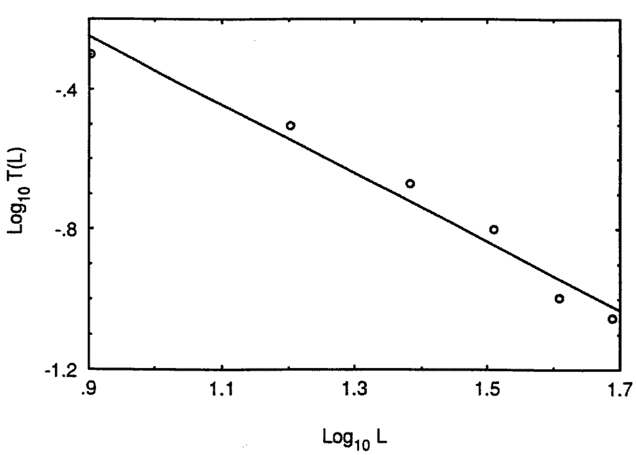


Figure 4. The transmission coefficient T versus the length of the disordered segment L, which consists of impurity spins $s = 2$ placed at random with probability $p = 0.6$. The soliton energy is $\epsilon = 1.625$.

4. Discussion

In summary, we have carried out numerical simulations on the propagation of solitons through a disordered segment in a classical Heisenberg model, which is integrable and has well-defined solutions without disorder. The reflected and transmitted solitons are found to exhibit robust features, and in the range investigated the transmission coefficient $T(\epsilon)$ decreases with the soliton energy ϵ. The elementary units in the scattering process are found to be the impurity bonds which each link two sites with different spins in the segment. The dependence of the transmission coefficient on the length of the disordered segment can fitted to a power law ($T(L) \propto L^{-1}$) defining an exponent close to -1 which has a long-tail behaviour indicating strong interference effects. We have also investigated the scattering of a soliton from a single impurity bond where the behaviour obtained is quite different, but the energy at which the transmission coefficient approaches to zero is almost the same as that in the case of a large segment. Our results also indicate important differences between the soliton propagation in random nonlinear spin systems and in elastic chains. It will be very interesting to consider in the future the question of quantum localization in the presence of non-linearity, a subject of current debate [15, 16].

Acknowledgments

This work was supported in part from a HCM network and by a ΠΕΝΕΔ Research Grant of the Greek Secretariat of Science and Technology. We thank Professor N Papanicolaou for introducing us to this problem, Dr A Mistriotis for discussions and a referee for a careful review and helpful comments.

References

[1] Evangelou S N and Katsanos D E 1992 *Phys. Lett.* **164A** 456
[2] Evangelou S N and Wang A Z 1993 *Phys. Rev.* B **47** 13 126
[3] Avgin I, Huber D L, and Ching W Y 1989 *Phys. Rev.* B **40** 4638
[4] Avgin I and Huber D L 1993 *Phys. Rev.* B **48** 13 625
[5] Pushkarov D I *et al* 1977 *Phys. Lett.* **61A** 339
[6] Cordeiro C E *et al* 1978 *Phys. Lett.* **66A** 332
[7] Haldane F D M 1982 *J. Phys. C: Solid State Phys.* **15** L1309
[8] Ishimori Y 1982 *J. Phys. Soc. Japan* **51** 3417
[9] de Azevedo L G, de Moura M A, Cordeiro C and Zeks B 1982 *J. Phys. C: Solid State Phys.* **15** 7391
[10] Papanicolaou N 1987 *J. Phys. A: Math. Gen.* **20** 3637
[11] Gredeskul S A and Kivshar Yu S 1992 *Phys. Rep.* **216** 1 and references therein
[12] Li Qiming, Soukoulis C M, Pnevmatikos St and Economou E N 1988 *Phys. Rev.* B **38** 11 888
[13] Kaup D J and Newell A C 1978 *Phys. Rev.* B **18** 5162
[14] Kaup D J and Newell A C 1978 *Proc. R. Soc.* A **361** 413
[15] Kivshar Yu S, Gredeskul S A, Sanchez A and Vazquez L 1990 *Phys. Rev. Lett.* **64** 1693
[16] Shepelyansky D L 1993 *Phys. Rev. Lett.* **70** 1787